

# **SOLID PHASE PYROLYSIS MODELING FOR FIRE DYNAMICS SIMULATOR FDS v5**

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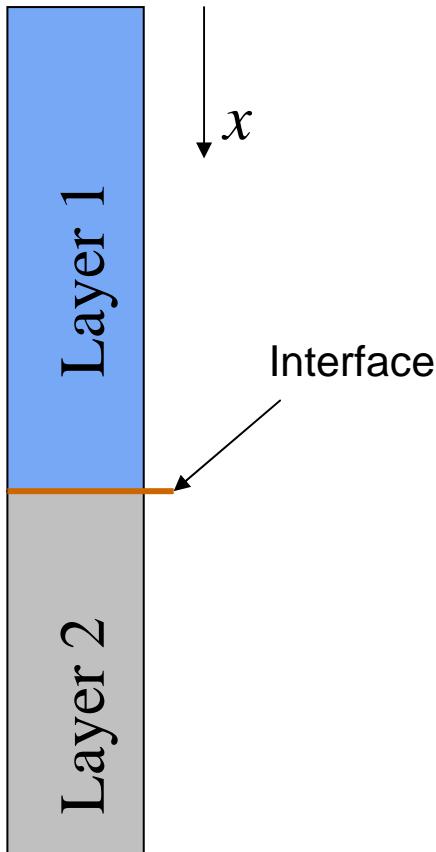


# OBJECTIVES OF THE NEW SOLID PHASE MODEL

- Layered materials
- Material mixtures
- Generalized way to model solid phase reactions
- Useful code for both engineers and researchers
- In-depth absorption of radiation
- Ease of use



# GOVERNING EQUATIONS



- Variables:  $T, \rho_i$
- 1D heat conduction equation

$$\overline{\rho c} \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x} k_s \frac{\partial T_s}{\partial x} + \dot{q}_s'''$$

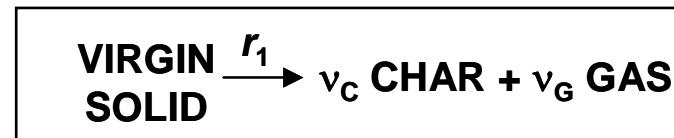
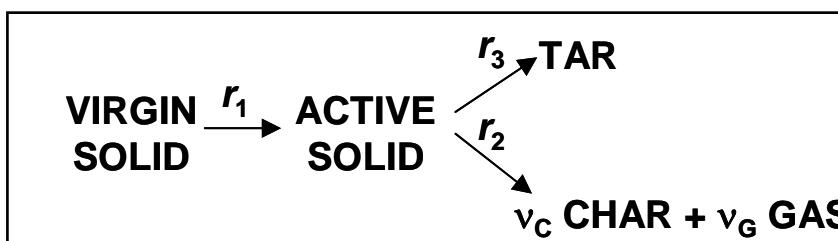
$$k_s = \sum_{i=1}^{N_m} X_i k_{s,i} \quad ; \quad \overline{\rho c} = \sum_{i=1}^{N_m} \rho_{s,i} c_{s,i} \quad ; \quad \dot{q}_s''' = \dot{q}_{s,c}''' + \dot{q}_{s,r}'''$$

$$\dot{q}_{s,c}''' = \sum_{k=1}^{N_m} \sum_{j=1}^{N_{r,k}} r_{kj} \left[ \Delta H_{kj} - \int_{T_0}^T (c_{s,k} - \nu_{s,kj} c_{s,p} - \nu_{f,kj} c_f - \nu_{w,kj} c_w) dT \right]$$

# VOLUMETRIC REACTIONS

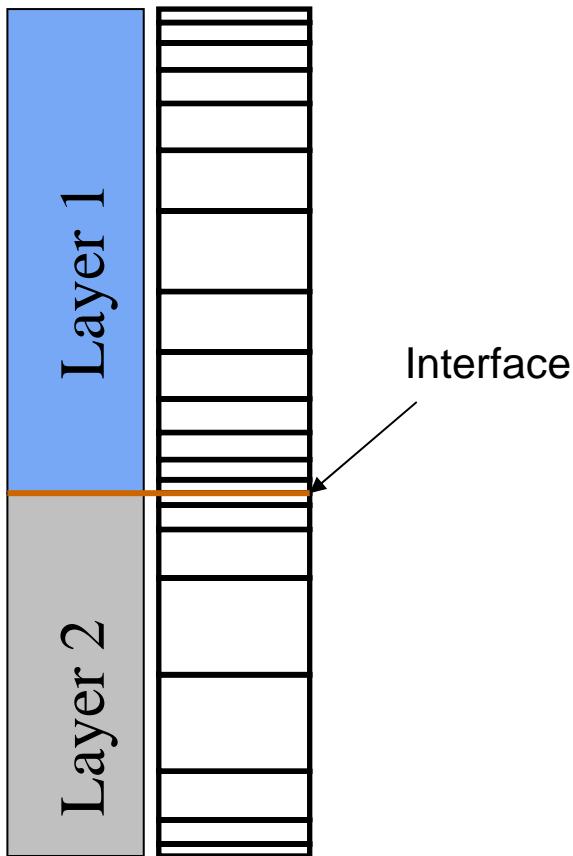
$$\frac{\partial}{\partial t} \left( \frac{\rho_i}{\rho_{i0}} \right) = - \sum_{j=1}^{N_i} r_{ij} + S_i \quad ; \quad r_{ij} = A_{ij} \cdot \left( \frac{\rho_i}{\rho_{i0}} \right)^{n_{ij}} \cdot e^{\left( -E_{A,ij} / RT_s \right)} \cdot \max[0, (T_s - T_{ign,ij})]^{n_{T,ij}}$$

- Arrhenius and power law dependence on temperature.
- Oxygen dependence not there yet in v5.0
- Used for both pyrolysis and evaporation reactions.
- Several simultaneous reactions possible.
- How to get *reaction path, A, E, ΔH,...*?



cellulose by Di Blasi 1998

# NUMERICAL SOLUTION

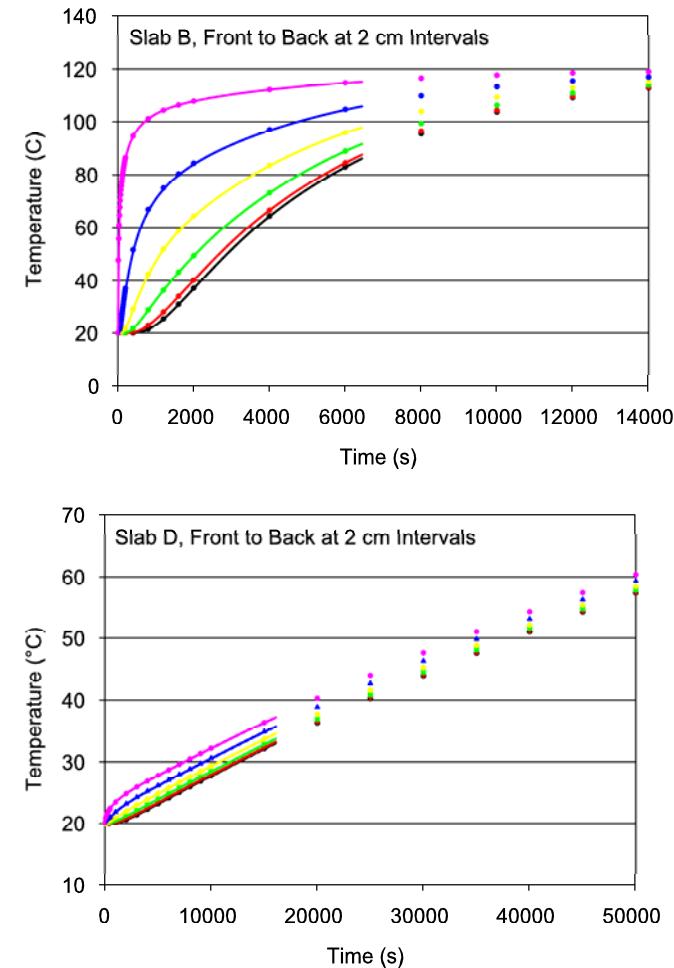
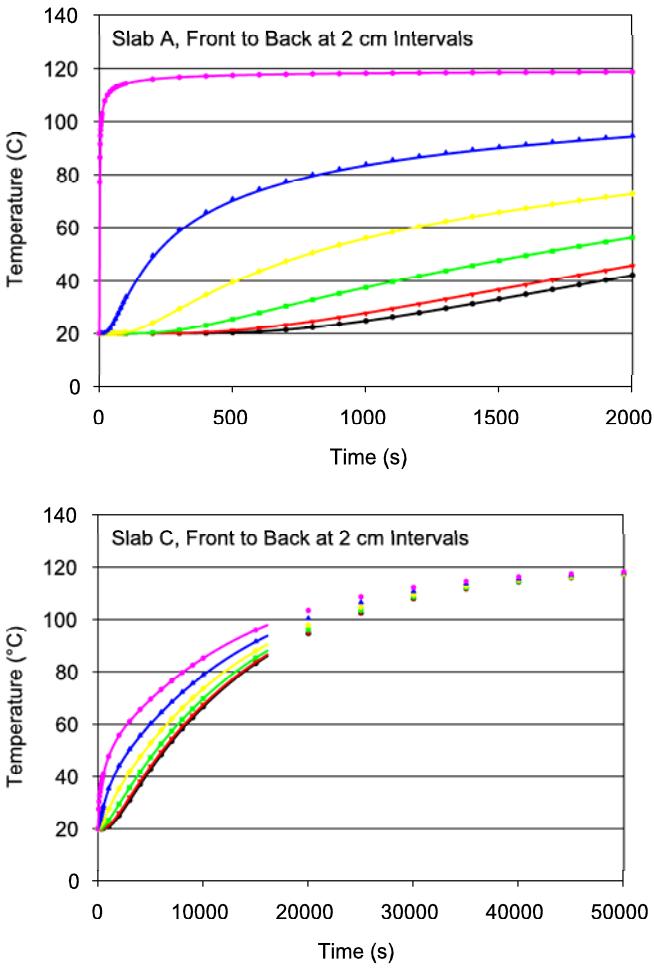


- Initially homogenous layers
- 1D difference method
- Refinement on layer interfaces and surfaces
- Symmetrical grids inside the layers
- Grids may shrink due to the reactions.

# VERIFICATION OF THE HEAT CONDUCTION

Comparison against  
analytical solutions of  
1D-conduction

	$Bi = hL/k$
Case A	100
Case B	10
Case C	1
Case D	0.1



# LAYER STRUCTURE

FDS 4



Back side BC

FDS 5



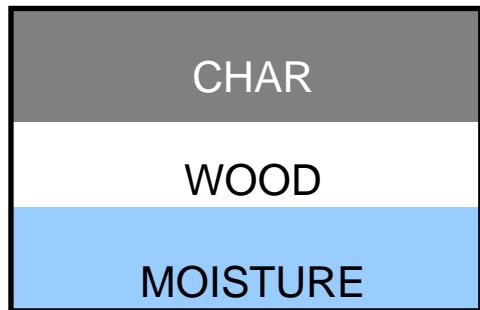
Back side BC



# MATERIAL MIXTURES AND REACTIONS

**FDS 4**

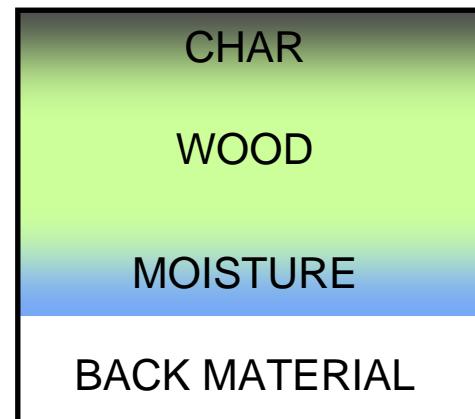
High heat flux approximation



BACK SIDE BC

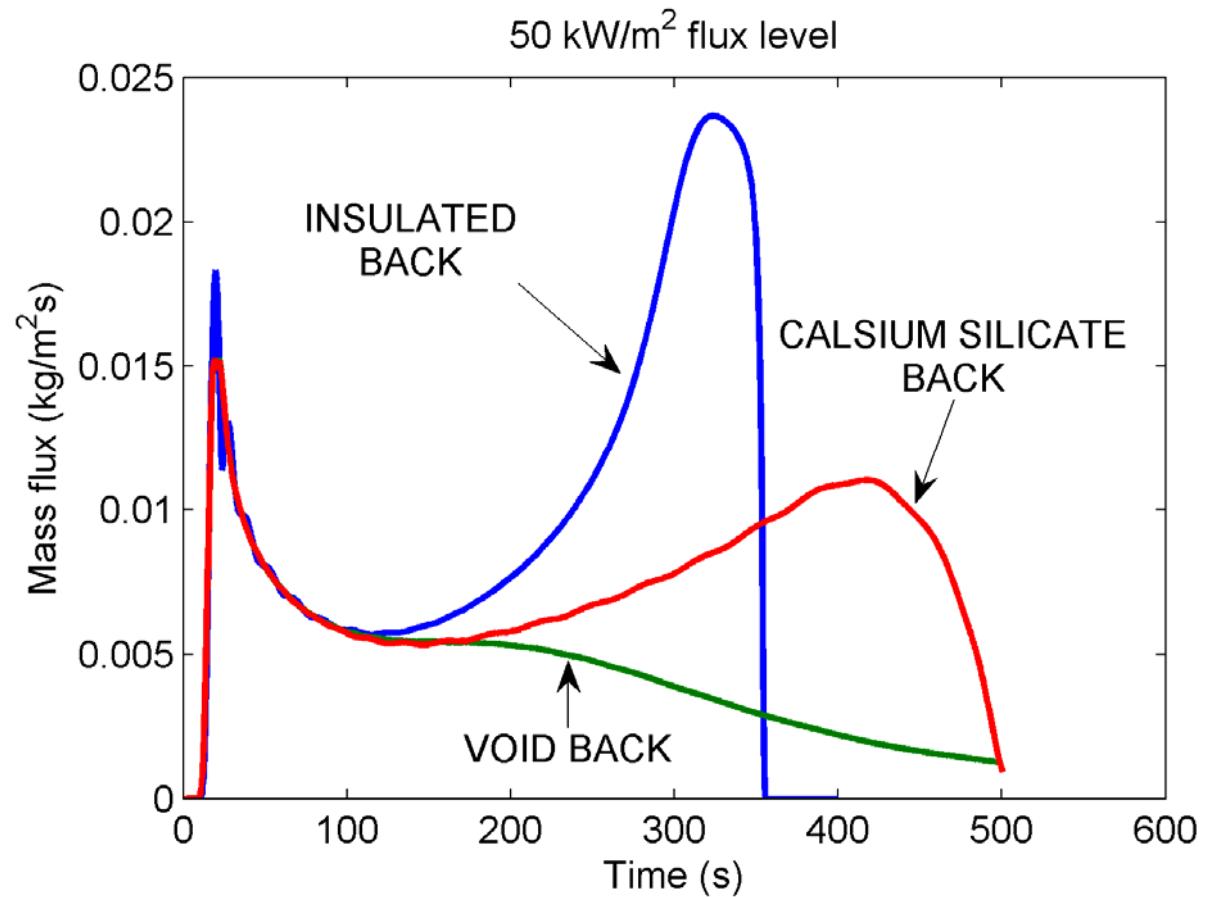
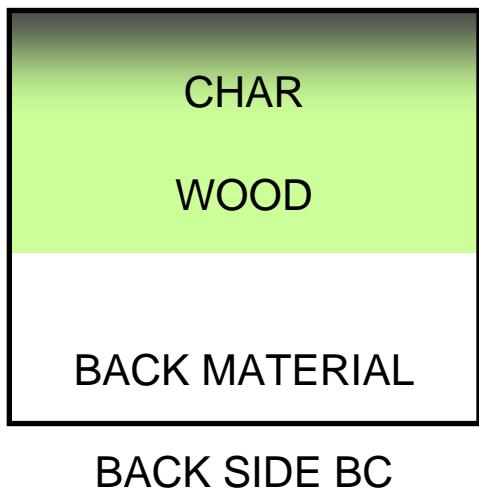
**FDS 5**

Generalized volumetric reactions



BACK SIDE BC

# LAYERS IN CONE CALORIMETER

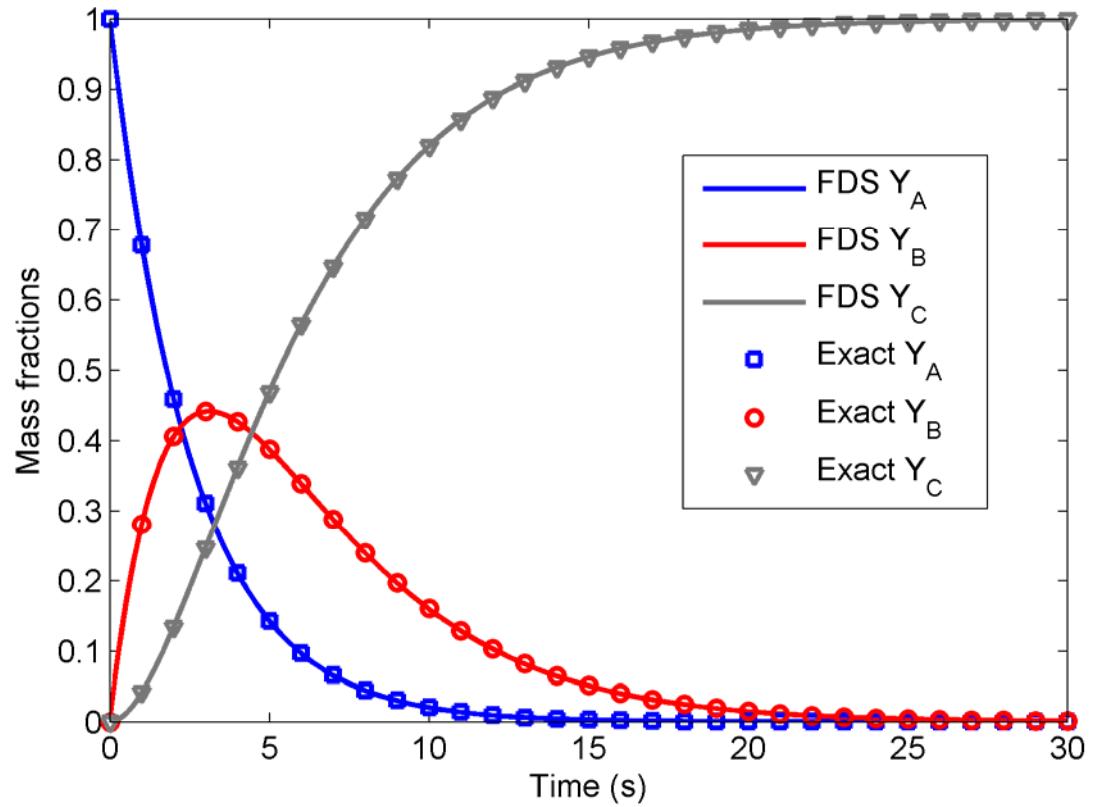


# VERIFICATION TEST OF SOLID PHASE REACTIONS

$$\frac{dY_a}{dt} = -K_{ab}Y_a$$

$$\frac{dY_b}{dt} = K_{ab}Y_a - K_{bc}Y_b$$

$$\frac{dY_c}{dt} = K_{bc}Y_a$$

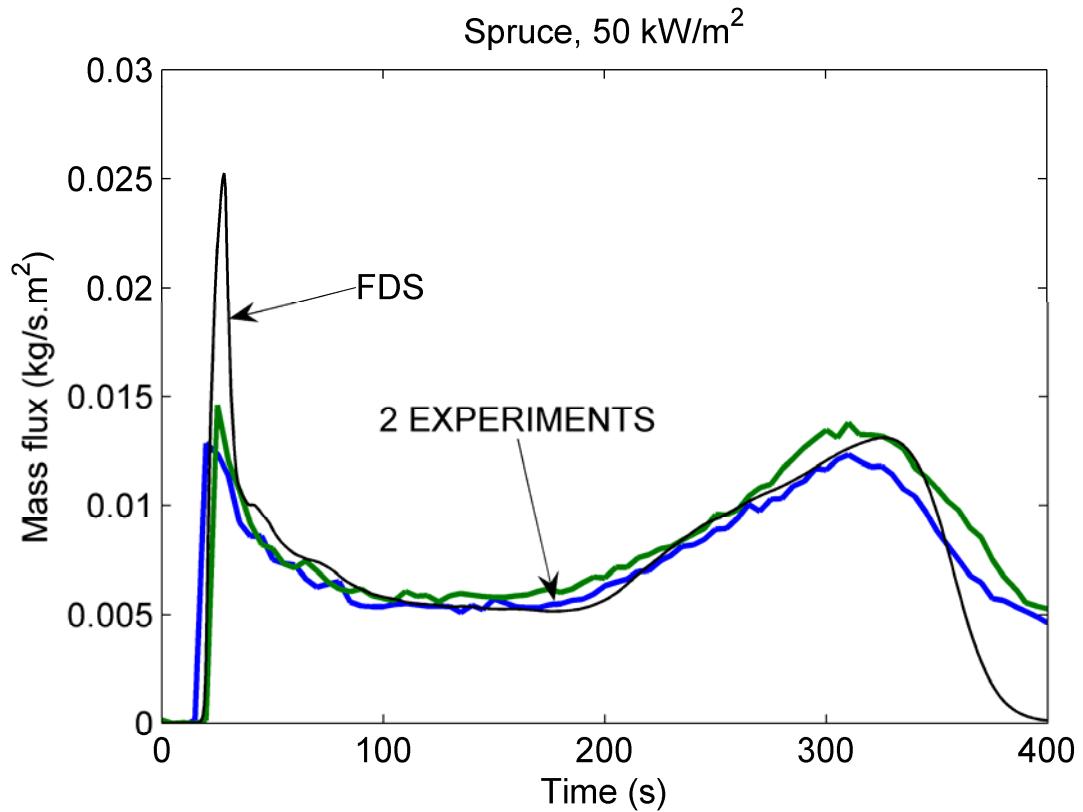
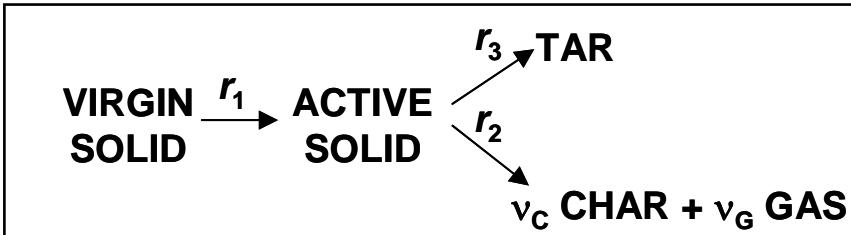


Exact solutions: C.Lautenberger, Univ. California

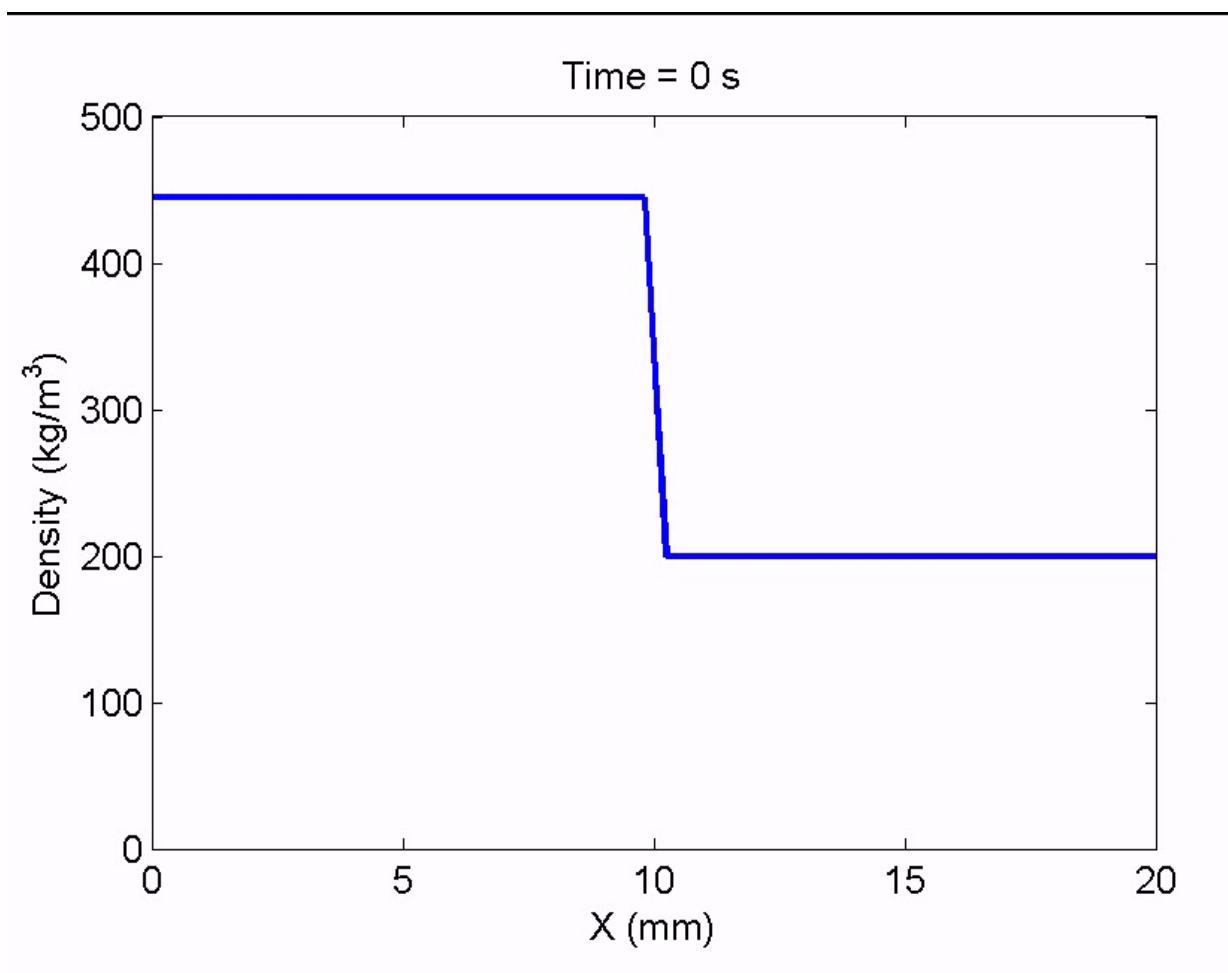


# 10 MM SPRUCE IN CONE CALORIMETER

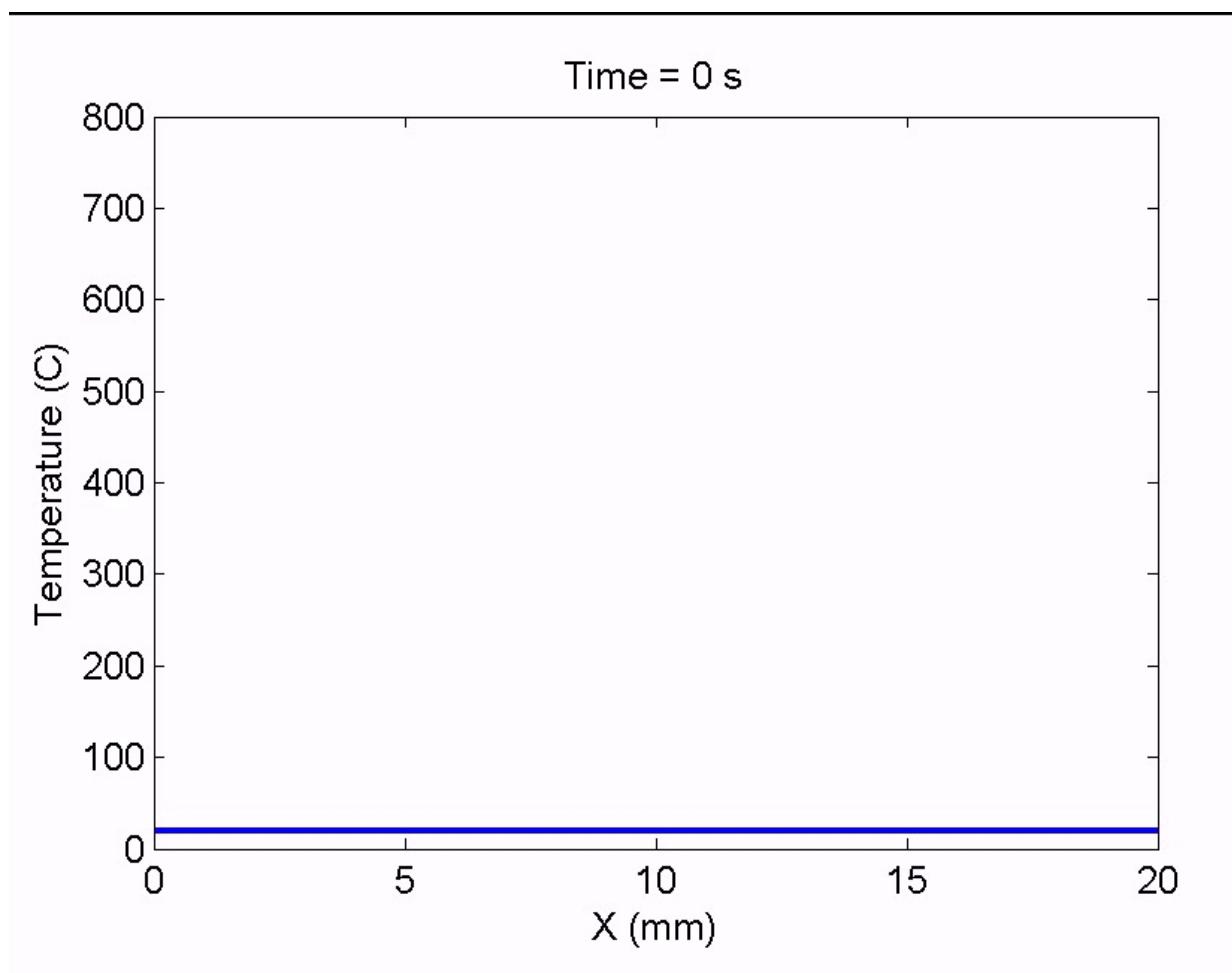
```
&SURF ID='SPRUCE'  
STRETCH_FACTOR = 1.  
CELL_SIZE_FACTOR = 0.5  
MATL_ID(1,:) = 'CELLU','water','lignin'  
MATL_MASS_FRACTION(1,:) = 0.7,0.1,0.2  
MATL_ID(2,:) = 'CASI'  
THICKNESS = 0.01,0.01 /
```



# DENSITY OF 10 MM SPRUCE (movie)

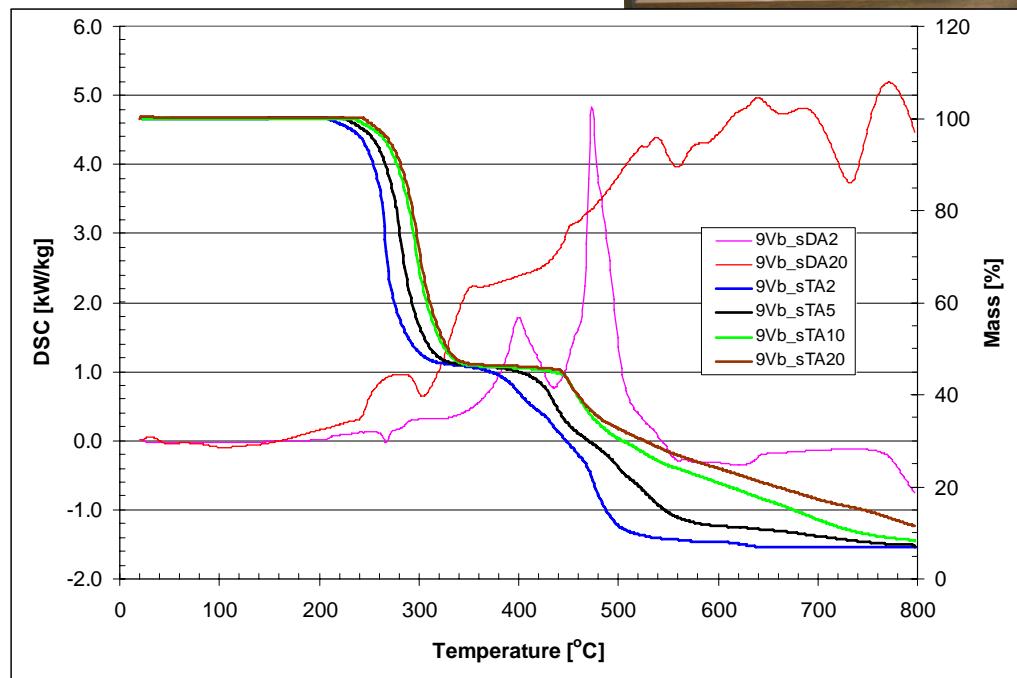
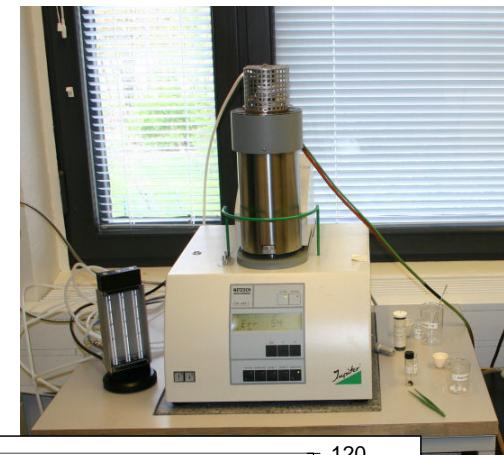


# TEMPERATURE OF 10 MM SPRUCE (movie)



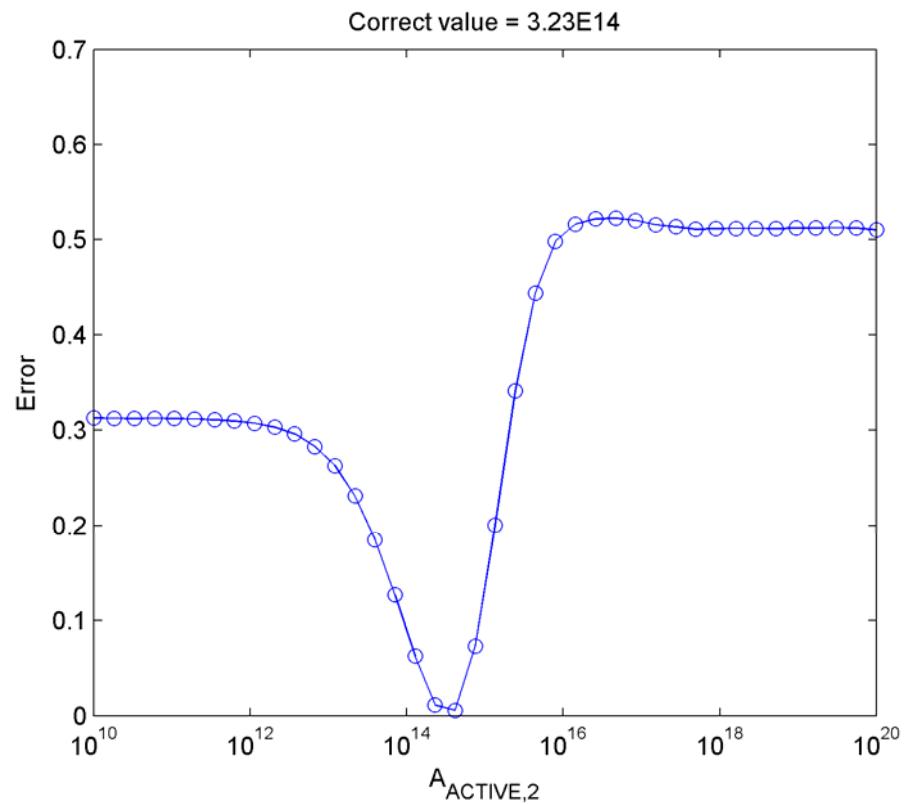
# HOW TO GET THE PARAMETERS?

- What we need?
  - reaction paths
  - rate coefficients ( $A, E, n$ )
  - reaction heats ( $\Delta H$ )
  - thermal properties
- Available measurements
  - Cone Calorimeter
  - TGA/DSC (= DTA)
  - Others
- What they measure? – Mass and energy



# SO - HOW TO GET THE PARAMETERS?

- Parameter estimation process:
  1. Model TGA or Cone with FDS
  2. Define error measure
  3. Minimize error
- Optimization problem
  - Multi-dimensional
  - Non-linear
  - Parameter ranges several orders of magnitude
  - Local minima
- Genetic algorithms have been suggested.



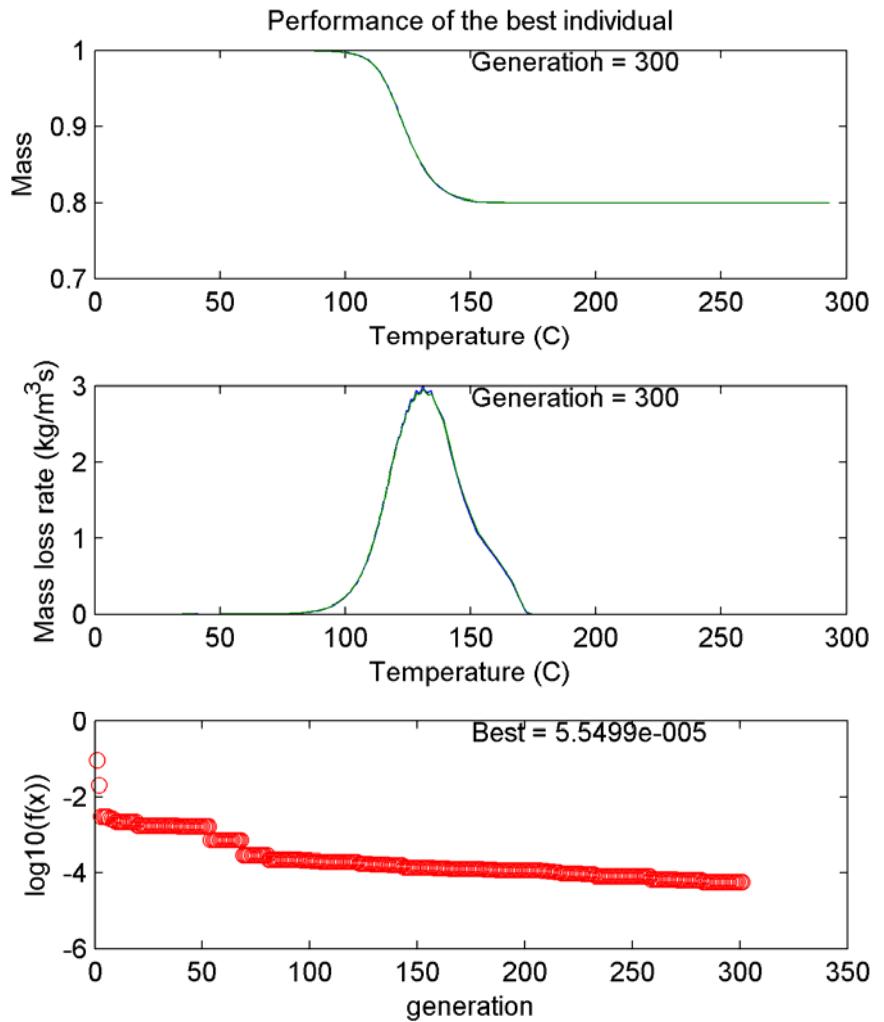
# LET'S TRY TO GET THE PARAMETERS

- Simulated test
- Single-step drying process

$$\dot{\rho}_w(t) = -A\rho_w(t) \exp(-E_A / RT_s)$$

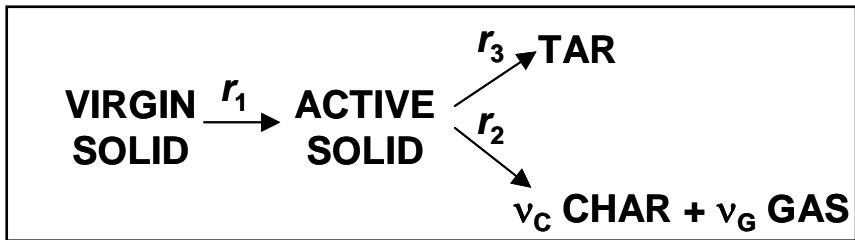
where  $A = 1E20$  1/s and  $E_A = 1.62E5$  J/mol.

- Error based on difference in mass and mass derivative time series.
- Genetic algorithm
  - MATLAB
  - GA Toolbox, Univ. Sheffield

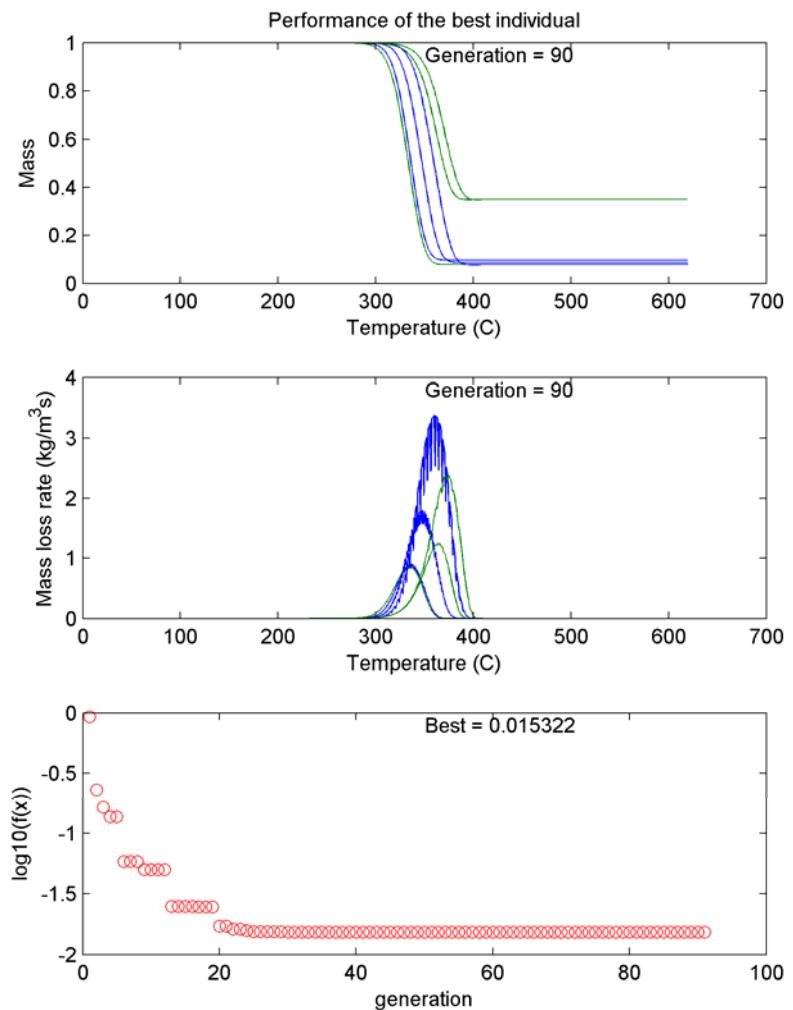


# LET'S TRY TO GET MORE PARAMETERS

- More complicated reaction



- Six parameters
- Three heating rates
- Simulated TGA data.
- Repeated runs of GA would produce different results
- Did not find the correct values.

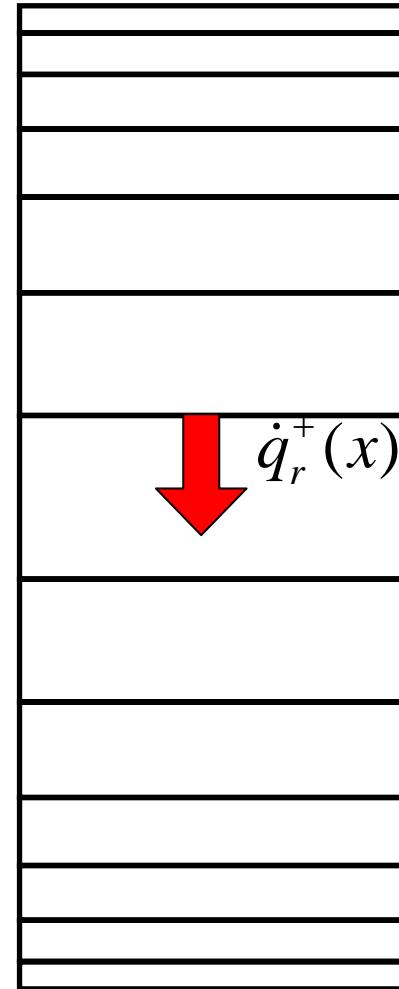


# RADIATION TRANSPORT IN-DEPTH

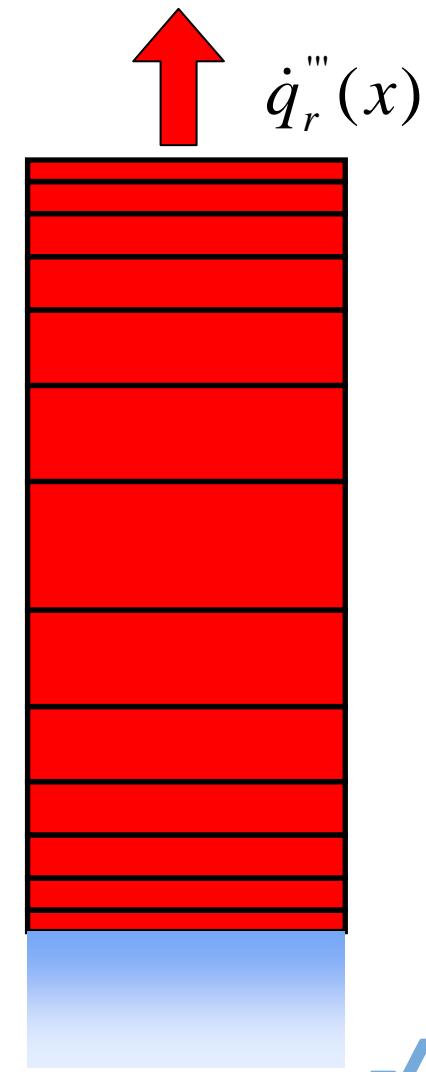
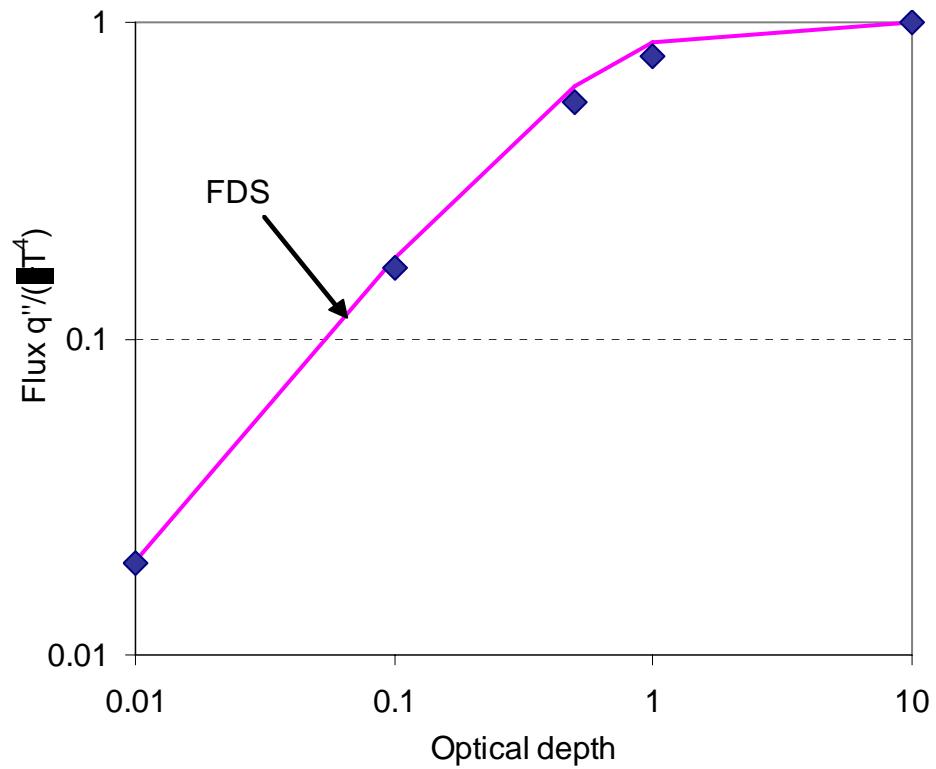
- FDS4: absorbtion at surface
- FDS5: transport inside the solid using two-flux method

$$\frac{1}{2} \frac{d\dot{q}_r^+}{dx} = \kappa_s (\sigma T^4 - \dot{q}_r^+) \quad (1)$$

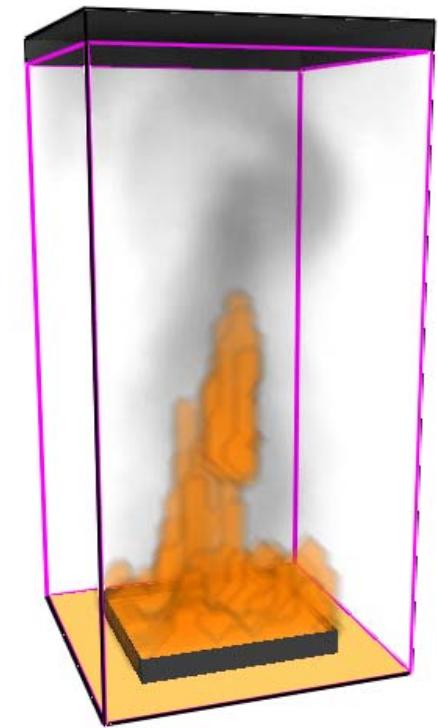
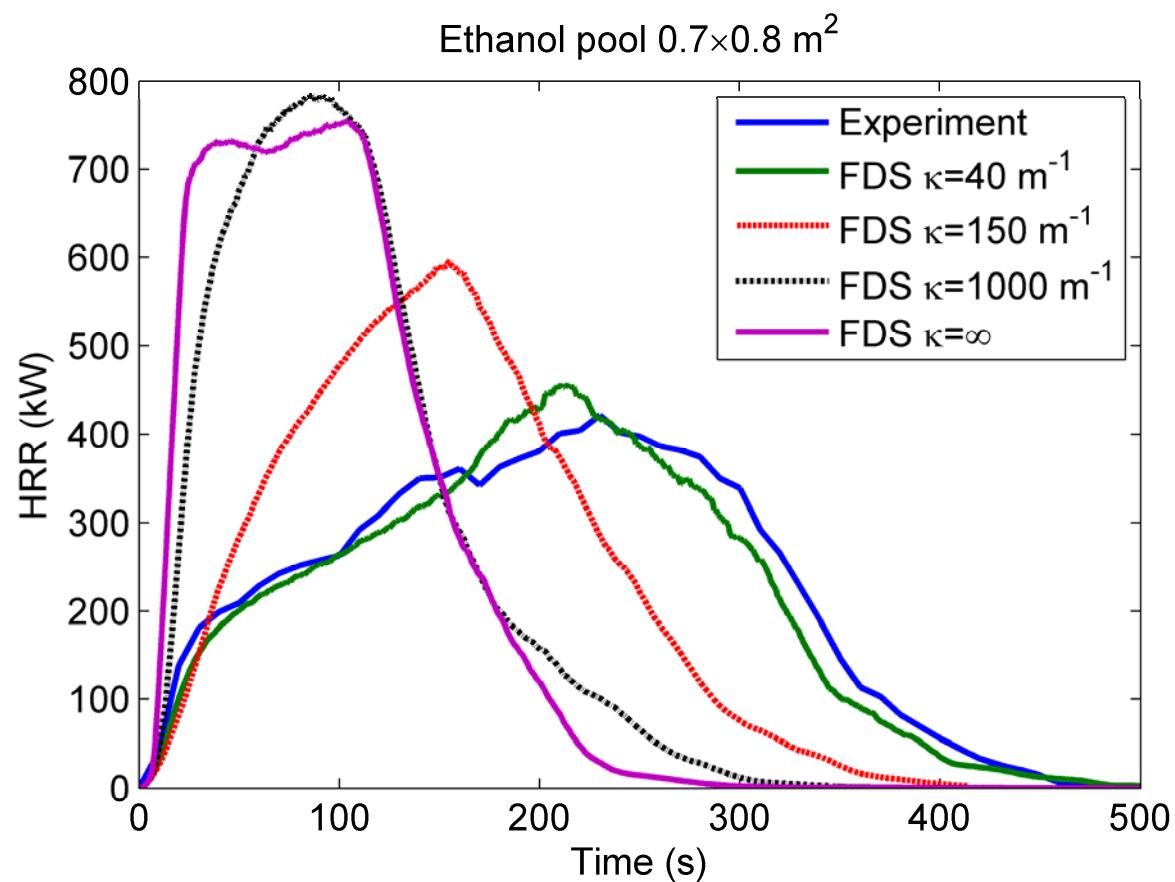
- One more material property:  
*solid (liquid) phase absorption coefficient*
  - Averaged over wave length



# VERIFICATION TEST OF IN-DEPTH RADIATION



# EFFECT OF IN-DEPTH RADIATION ON THE LIQUID POOL BURNING RATE



Experiment: Thomas, Moinuddin, Bennets (2005)

# SUMMARY

- New solid phase routine in FDS v5 allows the modeling of more complicated structures, materials and reactions.
- The same code can be used both by the engineers and the researchers.
- New heat transfer mechanism: internal radiation
  
- Need for validation and applications – do the volumetric reactions work in practice?
- Need for many new model parameters.
- Techniques to get the data are being developed.

